Structural and optical properties of $Zn_{1-x}Mg_xO$ layers grown by PA-MBE. Experiment vs. Theory

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Wurtzite $Zn_{1-x}Mg_xO$ and $Zn_{1-x}Cd_xO$ have been studied for over a decade. However, it should be emphasized that there is still a lack of detailed knowledge of many physical parameters for these materials. Knowledge of these properties is important in modeling and designing future devices. Nevertheless, the main parameters of the wurtzite MgO and CdO are not exactly known, as they are not stable in wurtzite structure.

The aim of our work was to determine experimentally basic properties of wurtzite $Zn_{1-x}Mg_xO$ layers and compare with the calculated values.

Our samples were grown by plasma-assisted molecular beam epitaxy on **a**-plane sapphire. The system was equipped with RF plasma cell as a source of gas and standard effusion cells for the group II elements. The growth was performed around 460ºC under nearly-stoichiometric conditions. The in-situ growth rate measured during epitaxy from optical reflectometry was at the level of 0.36 µm/h. A streaky pattern from the sample surface was revealed during and after sample growth by reflection high-energy electron diffraction (RHEED). Our samples were characterized by using various methods like atomic-force microscopy, absorption, photoluminescence, and X-ray diffraction. We also use different techniques (like X-ray diffraction and Rutherford backscattering spectrometry) to estimate the composition of Mg in $Zn_{1-x}Mg_xO$ layers.

Band structures of $Zn_{1-x}Mg_xO$ alloys were obtained by self-consistent ab-initio calculations based on the Local Density Approximation (LDA) to density functional theory. The relaxed atomic positions were determined by minimization of the Hellman-Feynman forces using pseudopotentials as implemented in the Vienna Ab-initio Simulation Package (VASP). Subsequently, in a second step of the calculations, the band structures were obtained by the Linear-Muffin-Tin-Orbital (LMTO) method in a full-potential (FP) version. A semi-empirical correction (LDA+C) for the deficiency of LDA in predicting semiconductor gaps was applied.

Experimentally obtained band gaps of $Zn_{1-x}Mg_xO$ for different magnesium concentrations, *x*, are in good agreement with the calculated values.